RKKY interaction between Ce ions in $Ce_xLa_{1-x}B_6$

P. Schlottmann

Department of Physics, Florida State University, Tallahassee, Florida 32306

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Ce ions in $(\text{Ce}_x \text{La}_{1-x}) B_6$ have a Γ_8 ground multiplet, which is fourfold degenerate and has orbital and spin content. The interaction between Ce ions is of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type, which competes with the Kondo screening. The conduction states of the compound are described by three approximately ellipsoidal pockets centered at the *X* points of the cubic lattice. The RKKY interaction is calculated considering the interference of the three pockets. The interaction strength strongly depends on the relative position of the ions, as well as on the relative orientation of the line joining two ions to the cubic crystalline field axis. The sixteen states of a pair of Ce ions are split by the RKKY interaction into a singlet, a triplet, and a twelvefold degenerate level. The ground state is always either a singlet or a triplet, depending on the sign of the interaction. Using the exact Bethe *ansatz* solution of a model for a pair of interacting impurities with Γ_8 ground multiplet, we calculate the occupation of the levels, the magnetic-field susceptibility, the specific-heat γ coefficient, and the Wilson ratio for the ground state as a function of the ratio of the RKKY soluting strength to the Kondo temperature along the main crystallographic directions. As a consequence of the RKKY splitting a pair of CeB₆ is also discussed.

I. INTRODUCTION

Heavy fermion systems at low temperatures and as a function of magnetic field, pressure, or alloying, may show a variety of phenomena, such as anomalous superconductivity, antiferromagnetism, ferromagnetism, quadrupolar order, non-Fermi-liquid properties, or just enhanced paramagnetism, all believed to arise from the band of heavy electrons. The origin of heavy electrons is the competition and interplay of strong local atomiclike Coulomb forces with the solid-state effects of the conduction band and the hybridization, which give rise to a 4f or 5f Kondoesque resonance at the Fermi level.

To explain the nonuniversal behavior of heavy fermion systems it is necessary to invoke at least two competing energy scales, e.g., the single site Kondo temperature and the Ruderman-Kittel-Kasuya-Yosida (RKKY) intersite interaction. While the single-impurity Kondo problem is by now well understood,¹⁻⁴ the Kondo lattice model still remains unsolved. The simplest model showing the competition of these two energy scales is the two-impurity Kondo problem, which for impurities of spin-1/2 has been studied by numerous methods,⁵ in particular by a Fermi-liquid approach,⁶ the numerical renormalization group,^{7,8} conformal field theory,⁹ and Bethe's ansatz.¹⁰ For strong ferromagnetic RKKY coupling between the impurities the spin screening occurs in two steps. The impurity spins first lock into a triplet state at intermediate temperatures, and are then spin compensated into a singlet state by the conduction electrons at low T in analogy to the S=1 two-channel Kondo problem.⁷ For strong antiferromagnetic RKKY coupling, on the other hand, the spins of the two impurities compensate each other by correlating antiferromagnetically, so that the Kondo effect only plays a secondary role. These two fixed points are in general joined by a line of fixed points^{8,9} yielding nonuniversal behavior as a function of RKKY coupling strength over T_K ,

except if the system has a special electron-hole symmetry built in. In the latter case the basins of attraction of the two stable fixed points (strong ferromagnetic and strong antiferromagnetic RKKY) are separated by an unstable fixed point with non-Fermi-liquid properties.⁸

The usual RKKY interaction refers to a parabolic band with a spherical Fermi surface. The band structure in realistic materials often differs considerably from a free-electron dispersion. For instance, the conduction states of the alloy $Ce_xLa_{1-x}B_6$ are characterized by three elliptic pockets centered at the *X* points of the cubic Brillouin zone¹¹⁻¹⁴ for the entire alloy range $0 \le x \le 1$. The contributions of these pockets to the RKKY interaction give rise to constructive and destructive interferences so that, depending on the relative position of the ions, the amplitude of the interaction is either enhanced or reduced. We study this interference in Sec. II.

Due to the orbital content of the f states the RKKY interaction is in general anisotropic, i.e., it depends on the relative orientation of the line joining the impurities to the crystallographic axis. In particular, for $Ce_xLa_{1-x}B_6$, the ground multiplet of the Ce ions is a Γ_8 quadruplet. The sixteen states describing a pair of Ce ions is split by the RKKY interaction into a singlet, a triplet, and twelvefold degenerated level. Depending on the sign of the interaction, the ground state is either a singlet or a triplet (see Sec. III). The Γ_8 ground state has quadrupolar content in addition to the spin magnetic moment. The interaction of impurities with Γ_8 ground state is of interest in view of the rich low-temperature phase diagram of the alloy series $Ce_xLa_{1-x}B_6$.¹⁵ Besides the paramagnetic Kondo-compensated phase, three additional phases involving long-range order of the antiferromagnetic and/or antiferroquadrupolar type have been found as a function of temperature, magnetic field, and concentration x.

In a recent publication we obtained the Bethe *ansatz* solution of a model for a pair of interacting impurities with Γ_8 ground multiplets.¹⁶ This exact solution was used in Ref. 16

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to study the situation of a RKKY interaction averaged over all directions that splits the 16 states into two multiplets of wave functions of even and odd parity with respect to the midpoint between the impurities. This simplified splitting scheme has the advantage that an analytic solution could be obtained. In Sec. IV we apply the Bethe *ansatz* solution of the model to investigate the consequences of the more realistic RKKY splitting into a singlet, a twelvefold degenerate manifold, and a triplet on the magnetic susceptibility, the specific-heat γ coefficient, the Wilson ratio, and the induced quadrupolar moment. Concluding remarks follow in Sec. V.

II. RKKY INTERACTION IN HEXABORIDES

The band structure of LaB_6 was calculated with variational methods¹¹ and the states close to the Fermi surface were found to be in good agreement with de Haas–van Alphen measurements.¹² The data are consistent with a set of three nearly spherical ellipsoids located at the *X* points of the cubic Brillouin zone. The intersections among the ellipsoids along the Γ -*M* lines are small and give rise to small necks. The Fermi surface of CeB₆ (Ref. 13) is very similar to that of LaB₆, leading to the conclusion that the additional *f* electron (the *f* level lies far below the Fermi energy) only contributes to a considerable enhancement of the effective mass.

Surprisingly, de Haas–Shubnikov oscillations could be observed for all *x* in $\operatorname{Ce}_{x}\operatorname{La}_{1-x}\operatorname{B}_{6}^{,14}$ revealing the existence of long-lived quasiparticles. The extremal cross-sectional areas of the Fermi surface interpolate smoothly between those of the two end compounds, while the effective mass is a maximum for $x \approx 0.9$. Hence, for the entire alloy regime the conduction states are given by three ellipsoids centered at the *X* points. We will neglect here the small overlaps of the ellipsoids.

We consider the following Anderson-like two-impurity Hamiltonian, $H=H_{cond}+H_{local}+H_V$,

$$H_{cond} = \sum_{\mathbf{k}\sigma j=1,2,3} \epsilon_{j}(\mathbf{k}) c_{j\mathbf{k}\sigma}^{\dagger} c_{j\mathbf{k}\sigma},$$

$$H_{local} = \sum_{l\sigma} \epsilon_{f} n_{l\sigma} + U \sum_{l} n_{l\uparrow} n_{l\downarrow},$$

$$H_{V} = V \sum_{il\mathbf{k}\sigma} (e^{i\mathbf{k}\cdot\mathbf{R}_{l}} d_{l\sigma}^{\dagger} c_{j\mathbf{k}\sigma} + \text{H.c.}), \qquad (1)$$

where $n_{l\sigma} = d_{l\sigma}^{\dagger} d_{l\sigma}$ is the number operator of the localized electrons, *U* is the intra-atomic Coulomb repulsion, ϵ_f the *f*-electron energy, and *V* the hybridization between the localized and conduction states. The two impurities are located at **R**_l, *l* = 1,2, and the dispersions of the ellipsoidal pockets are,

$$\epsilon_{1}(\mathbf{k}) = \frac{1}{2m} \left[\alpha^{2} \left(k_{x} - \frac{\pi}{a} \right)^{2} + \beta^{2} (k_{y}^{2} + k_{z}^{2}) \right],$$

$$\epsilon_{2}(\mathbf{k}) = \frac{1}{2m} \left[\alpha^{2} \left(k_{y} - \frac{\pi}{a} \right)^{2} + \beta^{2} (k_{x}^{2} + k_{z}^{2}) \right],$$

$$\epsilon_{3}(\mathbf{k}) = \frac{1}{2m} \left[\alpha^{2} \left(k_{z} - \frac{\pi}{a} \right)^{2} + \beta^{2} (k_{x}^{2} + k_{y}^{2}) \right],$$
 (2)

where α and β are dimensionless constants determining the effective mass and excentricity of the ellipsoids, and *a* is the lattice constant of the cube.

Firstly, the hybridization is eliminated via a Schrieffer-Wolff transformation, $e^{iS}He^{-iS}$, i.e., $H_V+i[S,H_{cond} + H_{local}]=0$, which is satisfied for¹⁷

$$iS = V \sum_{jl\mathbf{k}\sigma} \left[\frac{1 - n_{l-\sigma}}{\epsilon_j(\mathbf{k}) - \epsilon_f} + \frac{n_{l-\sigma}}{\epsilon_j(\mathbf{k}) - \epsilon_f - U} \right] \\ \times \left[e^{-i\mathbf{k}\cdot\mathbf{R}_l} c_{j\mathbf{k}\sigma}^{\dagger} d_{l\sigma} - e^{i\mathbf{k}\cdot\mathbf{R}_l} d_{l\sigma}^{\dagger} c_{j\mathbf{k}\sigma} \right].$$
(3)

The Hamiltonian to second order in V is now $H' = H_{cond} + H_{local} - i/2 [S, H_V]$. Assuming that there is always exactly one electron localized at each impurity and projecting all band energies onto the Fermi level, we obtain the Kondo Hamiltonian,¹⁷

$$H_{K} = J \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma' ljj'} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{l}} \mathbf{S}_{\sigma\sigma'} \cdot \mathbf{s}_{\sigma'\sigma} d^{\dagger}_{l\sigma} d_{l\sigma'} c^{\dagger}_{j\mathbf{k}\sigma'} c_{j'\mathbf{k}'\sigma},$$
(4)

where $J = -2V^2 U/[\epsilon_f (U + \epsilon_f)]$ is the antiferromagnetic exchange constant, and $\mathbf{S}_{\sigma\sigma'}$ and $\mathbf{s}_{\sigma'\sigma}$ are spin matrices for the impurities and the conduction electrons, respectively. Note that a conduction electron annihilated in one ellipsoidal pocket may reappear in another pocket. Due to the Kondo exchange the number of electrons in each ellipsoidal pocket is not conserved. This feature is the main difference with respect to the standard Kondo problem.

Secondly, the RKKY interaction between localized spins mediated by the conduction electrons is calculated to second order in the exchange coupling *J*. The two differences with the standard RKKY interaction are (i) the ellipsoidal character of the pockets and (ii) the fact that there are three bands. The general expression of the interaction between two spins, S_1 and S_2 , separated by the vector \mathbf{R}_{12} of components $n_x a$, $n_y a$, and $n_z a$ is

$$H_{RKKY} = \frac{J^2}{2} \mathbf{S}_1 \cdot \mathbf{S}_2 \sum_{jj'} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} f[\boldsymbol{\epsilon}_j(\mathbf{k})] \\ \times \operatorname{Re}[e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{12}}] / [\boldsymbol{\epsilon}_j(\mathbf{k}) - \boldsymbol{\epsilon}_{j'}(\mathbf{k}')].$$
(5)

Here Re denotes real part and f is the Fermi function.

We first assume that $\alpha = \beta$ (isotropic parabolic bands) and focus on the interference of the three bands. Two types of contributions have to be considered, namely, j=j' and $j \neq j'$. For j=j' we shift the integration variable to the center of the band and rescale $p = \alpha k$. With $p_F^2 = 2m\mu$ (μ being the chemical potential) we then obtain the standard result for each band

$$\frac{2mJ^2p_F^4}{(2\pi\alpha^2)^3}F(2p_F R_{12}/\alpha)\mathbf{S}_1\cdot\mathbf{S}_2,$$
(6)

where $F(x) = \cos(x)/x^3$ asymptotically for large *x*. For $j \neq j'$ the different centers of the ellipsoids (spheres) give rise to a phase factor that depends on the relative position of the impurity spins, e.g., $e^{i\pi(n_x-n_y)} = (-1)^{n_x+n_y}$ if j=1 and j'=2,

but otherwise the result is the same as Eq. (6). Hence, collecting all the terms, we obtain for isotropic bands

$$H_{RKKY} = \frac{2mJ^2 p_F^4}{(2\pi\alpha^2)^3} F(2p_F R_{12}/\alpha) \left(\sum_{jj'} (-1)^{n_j + n_{j'}}\right) \mathbf{S}_1 \cdot \mathbf{S}_2.$$
(7)

The new effect here is the interference, which gives rise to an enhancement factor of 9 if the n_j are either all even or all odd, but yields only 1 otherwise. Hence, the sites included on a super-bcc-lattice of lattice constant 2a interact particularly strongly, but their interaction with other sites is much weaker as a consequence of the interference.

Finally, we address the effects of the anisotropy of the bands. For this purpose we define,

$$R'_{1} = [(n_{x}/\alpha)^{2} + (n_{y}/\beta)^{2} + (n_{z}/\beta)^{2}]^{1/2}a,$$

$$R'_{2} = [(n_{y}/\alpha)^{2} + (n_{x}/\beta)^{2} + (n_{z}/\beta)^{2}]^{1/2}a,$$

$$R'_{3} = [(n_{z}/\alpha)^{2} + (n_{x}/\beta)^{2} + (n_{y}/\beta)^{2}]^{1/2}a,$$
(8)

in terms of which the three contributions for j=j' are

$$\frac{2mJ^2p_F^4}{(2\pi)^3\alpha^2\beta^4}\sum_j F(2p_FR_j')\mathbf{S}_1\cdot\mathbf{S}_2.$$
(9)

Similarly, for $j \neq j'$ we obtain

$$\frac{2mJ^2p_F^4}{(2\pi)^3\alpha^2\beta^4}(-1)^{n_j+n_{j'}}\frac{(R'_j+R'_{j'})^2}{4R'_jR'_{j'}} \times F[p_F(R'_j+R'_{j'})]\mathbf{S}_1\cdot\mathbf{S}_2,$$
(10)

and collecting all the terms we finally have

$$H_{RKKY} = \frac{2mJ^2 p_F^4}{(2\pi)^3 \alpha^2 \beta^4} \sum_{jj'} (-1)^{n_j + n_{j'}} \frac{(R'_j + R'_{j'})^2}{4R'_j R'_{j'}} \times F[p_F(R'_j + R'_{j'})] \mathbf{S}_1 \cdot \mathbf{S}_2.$$
(11)

This expression contains the interference between the three bands and the effects of the anisotropy. As a consequence of the latter (and disregarding the effect of the interference factor) the symmetry of the RKKY interaction is now cubic rather than spherical.

III. RKKY INTERACTION FOR Γ_8 STATES

So far we have considered the particularly simple situation of spin 1/2 impurities without orbital content, for which the RKKY interaction has the simple form $\vec{S}_1 \cdot \vec{S}_2$. As shown by Coqblin and Schrieffer¹⁸ for J=5/2 multiplets corresponding to Ce³⁺ ions ($M = -5/2, \ldots, 5/2$) the orbital angular momentum induces an anisotropy in the interaction, which asymptotically for large distances becomes

$$H_{RKKY} = \frac{m^* k_F^4 J^2}{\pi^3} \frac{\cos(2k_F R)}{(2k_F r)^3} \times \sum_{MM'} F(M) F(M') |1M, 2M'\rangle \langle 1M', 2M|,$$
(12)

where the bra and ket denote the impurity states and F(M) contains the anisotropy,

$$F(\pm \frac{1}{2}) = 3, \quad F(\pm \frac{3}{2}) = 0, \quad F(\pm \frac{5}{2}) = 0.$$
 (13)

Hence, only the components $M = \pm \frac{1}{2}$ can be interchanged. Here the axis of quantization is the line joining the impurities. The above results refer to a single isotropic parabolic band.

The situation is more complicated for a Γ_8 quartet, since there are now two directions involved, namely, the crystallographic axis and the line joining the impurities. With respect to the cubic axis the Γ_8 states for a J = 5/2 multiplet are

$$|\kappa\rangle = -\sqrt{\frac{1}{6}} |\frac{3}{2}\rangle - \sqrt{\frac{5}{6}} |-\frac{5}{2}\rangle, \quad |\lambda\rangle = |\frac{1}{2}\rangle,$$
$$|\mu\rangle = -|-\frac{1}{2}\rangle, \quad |\nu\rangle = \sqrt{\frac{5}{6}} |\frac{5}{2}\rangle + \sqrt{\frac{1}{6}} |-\frac{3}{2}\rangle. \tag{14}$$

If the line joining the impurities is parallel to the cubic axis, then the RKKY interaction between two impurities with Γ_8 ground multiplet is of the form of Eq. (12) with

$$F(\kappa) = F(\nu) = 0, \quad F(\lambda) = F(\mu) = 3, \tag{15}$$

so that again only the components $|\lambda\rangle$ and $|\mu\rangle$ can be exchanged. These states can be parametrized by a pseudospin 1/2 with components σ . The form of the RKKY interaction for **R**₁₂ parallel to the (1,0,0) direction is then

$$H_{RKKY} = 9 \frac{m^* k_F^4 J^2}{\pi^3} \frac{\cos(2k_F R)}{(2k_F r)^3} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2.$$
(16)

Hence, the 16 two-impurity states are split by the RKKY interaction into a singlet, a twelvefold degenerate multiplet (with zero energy) and a triplet. Depending on the sign of the interaction either the singlet or the triplet form the ground state.

For an arbitrary direction of \mathbf{R}_{12} with respect to the crystallographic axis the interaction Hamiltonian is more complicated. For each ion the four Γ_8 states can be written as linear combinations of the $|M\rangle$ states. A Kramers pair of them can be chosen such that they do not contain the states with M $=\pm 1/2$. We parametrize the other pair of Kramers states by a pseudospin 1/2 denoted with σ . Within this basis of states, only the σ doublets of the impurities can interact with each other. Hence, the general splitting scheme is again a singlet, a twelvefold degenerate multiplet and a triplet, and the expression of the interaction is again given by Eq. (16), except for a multiplicative factor in the amplitude arising from the projection of the σ states onto the $M = \pm 1/2$ states. For instance, for \mathbf{R}_{12} along the (1,1,1) direction the projection factor is 16/81 and if \mathbf{R}_{12} is parallel to the (1,1,0) direction it is $49/(16 \times 9)$.

Next we consider the interaction between impurities with a Γ_8 ground manifold mediated via three spherical electron

pockets centered at the X points of the cubic Brillouin zone. The procedure is the same as described in Sec. II and the interference of the three pockets again yields the phase factor $\sum_{ii'}(-1)^{n_j+n_{j'}}$ as for spin-1/2 impurities.

The anisotropy of the bands of $(La_xCe_{1-x})B_6$ does not affect the canonical transformation leading to the Coqblin-Schrieffer Hamiltonian, since as in Eq. (4) the energy of the conduction states is projected onto the Fermi level. The local symmetry at each Ce site is cubic, so that the partial-wave expansion can be done in terms of eigenstates of the cubic group. Alternatively, one can rescale k_x , k_y , and k_z for each pocket by α and β , as described in Sec. II, so that the effective symmetry of the bands becomes spherical. The integrals in the spin-correlation function of the conduction states between the two impurity sites are then evaluated as in Sec. II. The final result for the RKKY interaction is then

$$H_{RKKY} = A \frac{9mJ^2 p_F^4}{\pi^3 \alpha^2 \beta^4} \sum_{jj'} (-1)^{n_j + n_{j'}} \frac{(R'_j + R'_{j'})^2}{4R'_j R'_{j'}} \times F[p_F(R'_j + R'_{j'})] \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, \qquad (17)$$

where A is the constant containing the projection of the σ states onto the $M = \pm 1/2$ states discussed above.

In summary, we expect three effects for Ce ions in hexaborides beyond the usual RKKY interaction: (i) The interference of the three electron bands centered at the X points yields an enhancement factor of 9 if the n_j are either all even or all odd. (ii) The anisotropy of the bands introduces small modifications in the amplitude and in the period of oscillation. (iii) The 16 states constituting a pair of impurities with Γ_8 ground multiplet are split into a singlet, a twelvefold degenerate multiplet, and a triplet. The ground state is either the singlet or the triplet depending on the sign of the interaction. This holds for any direction of the line joining the impurity sites with respect to the crystal axis.

IV. PROPERTIES OF A PAIR OF INTERACTING IMPURITIES WITH Γ_8 STATES

In this section we discuss the two-impurity problem, in particular, the interplay of the RKKY splitting of the 16 states into a singlet, a twelvefold degenerate multiplet and a triplet with the Kondo screening. In a previous publication we outlined the Bethe *ansatz* solution of an integrable variant of the two-impurity Kondo problem.¹⁶ This solution was applied in Ref. 16 to a simpler splitting of the 16 states into two multiplets.

We first briefly summarize the conditions under which the model is integrable.¹⁶ (i) The impurities are Anderson-like with only the f^0 and f^1 configurations allowed. The localized electrons are considered in pairs, such that each impurity has one localized electron or they are both in the empty configuration. States with one impurity in the f^1 and the other one in the f^0 configurations are excluded. Since we are interested in the integer-valent limit, i.e., both impurities in the f^1 configuration, this assumption is not expected to have dramatic consequences. (ii) Since we have two impurities it is necessary to introduce two channels for the conduction electrons, one for each impurity or the even and odd parity states with respect to the midpoint between the impurity sites. This ap-

proximation is standard for numerical renormalization-group treatments.^{7,8} (iii) The two channels are sufficient to distinguish the impurities, so that both impurities can be considered effectively at the same site for the purpose of a "partialwave expansion." Both channels can now interact via a contact potential with the impurities. Without loss of generality, we can consider only forward moving particles along a ring with periodic boundary conditions and linearize the dispersion of the conduction states about the Fermi level. (iv) It is further imposed on the model that pairs of propagating electrons do not interchange individual electrons in the scattering process. In this way the set of incoming and outgoing pairs act like hard-core bosons and can only interchange their momentum.

The above variant of the two-impurity Kondo problem is integrable and can be mapped onto the N=16-fold degenerate Anderson impurity in the $U\rightarrow\infty$ limit,¹⁹ with the difference that the pairs act like hard-core bosons rather than fermions. This has no effect on the Bethe *ansatz* since also the multiple occupation of a hard-core boson is forbidden. The effective Hamiltonian is then

$$H_{eff} = -2i \sum_{m=1}^{N} \int dx b_{m}^{\dagger}(x) \frac{\partial}{\partial x} b_{m}(x) + 2\epsilon \sum_{m=1}^{N} |m\rangle \langle m|$$
$$+ V \sum_{m=1}^{N} \int dx \,\delta(x) (|m\rangle \langle 0|b_{m}(x) + \text{H.c.}), \qquad (18)$$

where b_m^{\dagger} creates a boson with component *m*. The bra and ket denote the impurity states. Here *V* is proportional but not identical to *V* in Eq. (1) and ϵ is related to ϵ_f . H_{eff} conserves the number of particles with given color *m*, $N_m = |m\rangle\langle m| + \int dx \ b_m^{\dagger}(x)b_m(x), \ m = 1, \dots, N$. (v) The RKKY interaction, crystalline, and the magnetic fields commute with Eq. (18) and can be incorporated *a posteriori* into the model. They just lift the *N*-fold degeneracy of the bosons.

A. Bethe *ansatz* equations

The Bethe *ansatz* solution of Hamiltonian (18) has been presented in Ref. 16. Here we limit ourselves to restate the ground-state equations in the integer-valent limit where each site has a magnetic moment (charge fluctuations are suppressed). The internal degrees of freedom are then described in terms of N-1 sets of rapidities. We denote with $\rho^{(l)}(\xi)$ and $\rho_h^{(l)}(\xi)$, $l=0, \ldots, N-2$, the distribution functions of the "particles" and "holes" within those sets. The density functions satisfy the following Wiener-Hopf integral equations,¹⁹

$$\rho_{h}^{(l)}(\xi) + \sum_{q=0}^{N-2} \int_{-\infty}^{B_{q}} d\xi' \rho^{(q)}(\xi') G_{l+1,q+1}^{\exp}(\xi - \xi')$$

= $F_{N-l-1}(\xi - \epsilon),$ (19)

where $G_{l+1,q+1}^{exp}(\xi)$ and $F_m(\xi)$ are the Fourier transforms of

$$\hat{G}_{l,q}^{\exp}(\omega) = \exp(|\omega|V^2/4) \frac{\sinh[\omega V^2 \min(l,q)/4]}{\sinh(\omega V^2/4)}$$

$$\times \frac{\sinh\{\omega V^2[N - \max(l,q)]/4\}}{\sinh(N\omega V^2/4)},$$

$$\hat{F}_m(\omega) = \frac{\sinh(m\omega V^2/4)}{\sinh(N\omega V^2/4)}.$$
(20)

This set of equations holds for $l=0, \ldots, N-2$. The densities for the host satisfy similar relations but with $\epsilon = 0$. Unless specified by a subscript "*host*," the densities refer to the impurity. The integration limits B_l correspond to the Fermi points of each class of states and are determined by the number of particles of each "color" N_l through

$$\int_{-\infty}^{B_l} d\xi \rho_{host}^{(l)}(\xi) = N_{l+1} - N_{l+2}.$$
(21)

The population differences of the impurity levels is given by a similar relation involving the density functions of the impurities.

B. Splitting scheme

We assume that the bandwidth is much larger than the Kondo temperature, the RKKY splitting, and all other mechanisms lifting the spin degeneracy. First we consider the N=16-fold multiplet split by the RKKY interaction into a singlet, a twelvefold multiplet, and a triplet. We parametrize the splitting energies by 3Δ and Δ , respectively. Two situations have to be distinguished, since depending on the sign of the RKKY interaction either the singlet or the triplet can have the lowest energy. This generalizes the splitting into singlet and triplet states for a pair of spin-1/2 impurities.

For antiferromagnetic coupling between the impurities, $\Delta > 0$, the difference in population of the singlet and one of the states of the twelvefold multiplet is given by $\rho^{(0)}$ and the occupation difference between one of the states of the twelvefold multiplet and one of the triplet states by $\rho^{(12)}$. Hence, $B_1 = -\infty$ for all *l* except B_0 and B_{12} , which are finite and determined by Δ . The difference $B_0 - B_{12}$ is constant and is obtained numerically to be 0.851. The natural energy scale of the model is the Kondo temperature for the Coqblin-Schrieffer model with *N* degrees of freedom, T_K $= D \exp[(4\pi\epsilon)/(NV^2)]$, where *D* is a cutoff for the electronic excitations introduced *a posteriori* into the Bethe *ansatz*.⁴

The problem for $\Delta > 0$ is now reduced to the solution of two coupled Wiener-Hopf equations, which is obtained numerically. The integration kernels and the driving terms in Eq. (19) can be expressed in terms of digamma functions. Denoting with n_s , n_d , and n_t the population of one state corresponding to the singlet, the twelvefold degenerate multiplet and the triplet, respectively, we have from the completeness condition that $n_s + 12n_d + 3n_t = 1$. These level occupations are shown in Fig. 1 as a function of Δ/T_K . For zero splitting all levels have the same occupation and as Δ/T_K becomes very large n_s asymptotically (on a logarithmic scale) tends to 1, while n_d and n_t asymptotically approach zero.

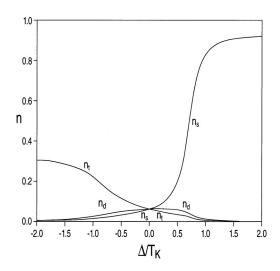


FIG. 1. Occupation per state for a pair of Γ_8 impurities split into a singlet (n_s) , a twelvefold degenerate multiplet (n_d) , and a triplet (n_t) as a function of Δ/T_K in the ground state.

For ferromagnetic coupling between the impurities, $\Delta <0$, the difference in population of one of the triplet states and one of the states of the twelvefold multiplet is given by $\rho^{(2)}$ and the occupation difference between one of the states of the twelvefold multiplet and the singlet is given by $\rho^{(14)}$. Hence, all $B_1 = -\infty$, except for B_2 and B_{14} , which are parametrized by Δ and $B_2 - B_{14} = -0.851$. The problem again consists of the numerical solution of two coupled Wiener-Hopf equations and the results for n_s , n_d , and n_t are shown in Fig. 1. For zero splitting, all levels have the same occupation, and as Δ/T_K tends to $-\infty$, n_t approaches the value 1/3, while n_d and n_t tend to zero. For large Δ/T_K the dependence is on a logarithmic scale, which is characteristic of asymptotic freedom.

C. Magnetic susceptibility

The susceptibility is obtained as the linear response of the impurities to a small homogeneous field. The magnetic field lifts the degeneracy of the triplet and the twelvefold multiplet, so that now all integration limits B_l are finite. We assume that $H \ll |\Delta| \ll D$, so that in Eq. (19) for antiferromagnetic RKKY coupling we have that $B_l \ll B_0$ for all $l \neq 0,12$, which are the ones parametrizing the Zeeman splitting. In linear response, the feedback of $\rho^{(l)}$ for $l \neq 0,12$ on the distribution functions $\rho^{(0)}$ and $\rho^{(12)}$ can be neglected,^{4,19} so that we can use the solution for $\rho^{(0)}$ and $\rho^{(12)}$ of the previous subsection. The ratio of the susceptibilities of the impurity and the host is then given by the $\xi \rightarrow -\infty$ asymptote of the driving terms for $\rho^{(l)}$ for $l \neq 0,12$.

Eliminating $\rho^{(0)}$ and $\rho^{(12)}$ from Eq. (19), we obtain after some algebra, that the asymptotic dependence of the driving terms for $\xi \rightarrow -\infty$ is

$$(1/6V^{2})\sin(\pi l/12)\exp(\pi\xi/6V^{2})$$
$$\times [\hat{\rho}_{h}^{(0)}(i\pi/6V^{2}) + \hat{\rho}_{h}^{(12)}(i\pi/6V^{2})], \qquad (22)$$

for $l = 1, \ldots, 11$, while for l = 13, 14 we obtain

$$(1/\sqrt{3}V^2)\exp(2\pi\xi/3V^2)\hat{\rho}_h^{(12)}(i2\pi/3V^2),$$
 (23)

where the *hat* denotes a Fourier transform. Note that because the singlet has lowest energy, in this case there is no driving term of the Kondo type.

The matrix elements of the Zeeman energy for the Γ_8 quartet are used to obtain the effective magnetic moments of the triplet and the twelvefold multiplet. We limit ourselves to study the susceptibility for impurities joined by a line parallel to the (1,0,0) and (1,1,1) directions,

$$\chi_{imp}^{s} = \frac{502}{9D} A_{12} + \frac{18}{9D} A_{3}, \quad \mathbf{R} \| (1,0,0),$$
$$\chi_{imp}^{s} = \frac{422}{9D} A_{12} + \frac{98}{9D} A_{3}, \quad \mathbf{R} \| (1,1,1), \quad (24)$$

where

$$A_{12} = \frac{\hat{\rho}_{h,imp}^{(0)}(i\pi/6V^2) + \hat{\rho}_{h,imp}^{(12)}(i\pi/6V^2)}{\hat{\rho}_{h,host}^{(0)}(i\pi/6V^2) + \hat{\rho}_{h,host}^{(12)}(i\pi/6V^2)},$$

$$A_3 = \frac{\hat{\rho}_{h,imp}^{(12)}(i2\pi/3V^2)}{\hat{\rho}_{h,host}^{(12)}(i2\pi/3V^2)}.$$
(25)

Here we explicitly identified the host and impurity densities with a subscript. The corresponding expressions are the same except that for the host $\epsilon = 0$ or $T_K = D$.

Similarly, for ferromagnetic RKKY coupling, a small magnetic field lifts all degeneracies, so that $B_l \ll B_{14}$ for all $l \neq 2,14$. Again, in linear response, the feedback of $\rho^{(l)}$ for $l \neq 2,14$ on the distribution functions $\rho^{(2)}$ and $\rho^{(14)}$, can be neglected^{4,19} so that we can use the solution for $\rho^{(2)}$ and $\rho^{(14)}$ of the previous subsection. The $\xi \rightarrow -\infty$ asymptotes of the driving terms for $\rho^{(l)}$ for $l \neq 2,14$ are now

$$(1/\sqrt{3}V^2)\exp(2\pi\xi/3V^2)$$

 $\times [\exp(-2\pi\epsilon/3V^2) + \hat{\rho}_k^{(2)}(i2\pi/3V^2)], (26)$

for l = 0, 1, and for l = 3, ..., 13

$$(1/6V^{2})\sin[\pi(l-2)/12]\exp(\pi\xi/6V^{2})$$
$$\times [\hat{\rho}_{h}^{(2)}(i\pi/6V^{2}) + \hat{\rho}_{h}^{(14)}(i\pi/6V^{2})], \qquad (27)$$

and the magnetic susceptibility is given by Eq. (24) with A_3 and A_{12} being replaced by C_3 and C_{12} , respectively,

$$C_{12} = \frac{\hat{\rho}_{h,imp}^{(2)}(i\pi/6V^2) + \hat{\rho}_{h,imp}^{(14)}(i\pi/6V^2)}{\hat{\rho}_{h,host}^{(2)}(i\pi/6V^2) + \hat{\rho}_{h,host}^{(14)}(i\pi/6V^2)},$$

$$C_3 = \frac{\exp(-2\pi\epsilon/3V^2) + \hat{\rho}_{h,imp}^{(2)}(i2\pi/3V^2)}{1 + \hat{\rho}_{h,host}^{(2)}(i2\pi/3V^2)}.$$
(28)

Since the triplet has lowest energy, C_3 has a Kondo driving term corresponding to a spin-1.

The logarithm of the homogeneous field susceptibility for the impurity normalized to $\chi_{imp}(\Delta=0)=520/(9T_K)$ is shown in Fig. 2. The susceptibility is always finite because due to the Kondo effect the ground state is always a singlet. For antiferromagnetic RKKY interaction χ_{imp}^{s} dramatically decreases with Δ , because the impurities are locked into a

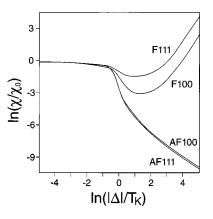


FIG. 2. Logarithm of the uniform magnetic-field susceptibility normalized to its $\Delta = 0$ value as a function of $\ln(|\Delta|/T_K)$ for the ground state for ferromagnetic and antiferromagnetic RKKY coupling. Here the vector **R** joining the two impurities is along the (1,0,0) and (1,1,1) directions of the crystal. For sufficiently large $\Delta > 0$ we obtain that χ^s_{imp} drastically decreases as a consequence of the formation of the singlet state between the impurities, while for $\Delta < 0$ the susceptibility increases with a power of $|\Delta|/T_K$ due to the Kondo effect of the triplet states.

singlet, compensating each other. This result is essentially independent of the orientation of **R** with respect to the crystal axis. For ferromagnetic RKKY, on the other hand, the Kondo effect corresponding to a triplet develops. This is seen by the straight-line asymptotes on the log-log plot. Although there are some analogies to a pair of spin-1/2 impurities, the quantitative outcome for impurities with a Γ_8 ground state is very different because of the presence of the twelvefold degenerate multiplet.

D. Low-temperature specific heat

The low-temperature specific heat is proportional to *T*. The γ coefficient is obtained via a Sommerfeld expansion and is given by²⁰

$$\gamma_{imp} = \frac{\pi}{6} \sum_{l=0}^{N-2} \rho_{imp}^{(l)}(B_l) / \rho_{host}^{(l)}(B_l).$$
(29)

In zero magnetic field and for antiferromagnetic RKKY interaction, this expression reduces to

$$\gamma_{imp} = \frac{\pi}{6} \left[11A_{12} + 2A_3 + \frac{\rho_{imp}^{(0)}(B_0)}{\rho_{host}^{(0)}(B_0)} + \frac{\rho_{imp}^{(12)}(B_{12})}{\rho_{host}^{(12)}(B_{12})} \right].$$
(30)

The former two terms are contributions from the spin fluctuations whithin the twelvefold multiplet and the triplet (see susceptibility), while the last two terms arise from the RKKY splitting and correspond to thermal fluctuations of the populations of the multiplets.

Similarly, for ferromagnetic RKKY interaction, Eq. (29) reduces to

$$\gamma_{imp} = \frac{\pi}{6} \left[11C_{12} + 2C_3 + \frac{\rho_{imp}^{(2)}(B_2)}{\rho_{host}^{(2)}(B_2)} + \frac{\rho_{imp}^{(14)}(B_{14})}{\rho_{host}^{(14)}(B_{14})} \right].$$
(31)

The physical origin of the terms is the same as in Eq. (30). Note that in the limit $\Delta \rightarrow 0$ both expressions become $\gamma_{imp} = (\pi/6)(N-1)/T_K$. The logarithm of the γ coefficient nor-

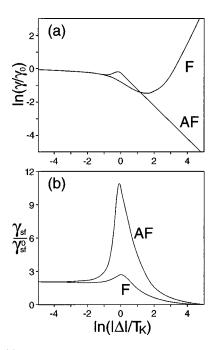


FIG. 3. (a) Logarithm of the low-temperature specific-heat γ coefficient normalized to its value for $\Delta = 0$ as a function of $\ln(|\Delta|/T_K)$. (b) Contribution of the thermal fluctuations between the multiplets, given by the last two terms in Eqs. (30) and (31), respectively, and normalized to the value of one of them for $\Delta = 0$.

malized to its value for $\Delta = 0$ is displayed in Fig. 3(a) as a function of $\ln(|\Delta|/T_K)$. For antiferromagnetic RKKY coupling, the γ coefficient is strongly suppressed by the formation of the singlet between the two impurities, while for ferromagnetic coupling the Kondo effect of the triplet leads to a dramatic enhancement for large $|\Delta|/T_K$. This is seen in the log-log plot as a straight line.

The spin fluctuations within the multiplets, given by the terms A_3 , A_{12} , C_3 , and C_{12} , are the same ones contributing to the susceptibility. The thermal fluctuations between the multiplets, given by $\rho_{imp}^{(l)}(B_l)/\rho_{host}^{(l)}(B_l)$ for l=0,12 and l=2,14, respectively, are displayed in Fig. 3(b). As a function of $\ln(|\Delta|/T_K)$ this contribution has a resonance shape at about $|\Delta| \approx T_K$. For larger values of $|\Delta|$ the contributions are quenched by the splitting. For $\Delta=0$ the expression is normalized to two, because two sets of rapidities contribute to the splitting.

The Wilson ratio, $W = \chi_{imp}^S / \gamma_{imp}$, normalized to its $\Delta = 0$ value, is shown in Fig. 4. Its $\ln(|\Delta|/T_K)$ -dependence evidences the nonuniversal nature of the interplay between RKKY and Kondo interactions. For sufficiently large $|\Delta|$ only the spin fluctuations contribute to γ_{imp} so that W approaches a constant given by the Curie constant of the ground multiplet.

E. Quadrupolar moment

The orbital content of the Γ_8 states and the RKKYinteraction splitting of the 16 states always induce a quadrupolar polarization Q. For simplicity the quadrupolar field is chosen parallel to the axis of quantization, i.e., coupling to each impurity with the operator $J_z^2 - J(J+1)/3$, where J= 5/2. This operator is diagonal in the Γ_8 basis, Eq. (14). Using the matrix elements of the quadrupolar operator for

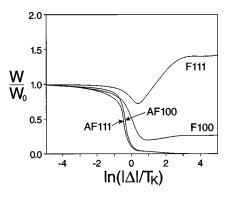


FIG. 4. Wilson ratio defined as $W(\Delta) = \chi^s_{imp} / \gamma_{imp}$ normalized to its value for $\Delta = 0$ as a function $\ln(|\Delta|/T_K)$ for the ground state. The Wilson ratio is nonuniversal and saturates for large $|\Delta|$. Ferromagnetic and antiferromagnetic RKKY coupling is considered and the vector **R** joining the two impurities is along the (1,0,0) and (1,1,1) directions of the crystal.

the Γ_8 states we obtain for antiferromagnetic and ferromagnetic RKKY coupling, respectively,

$$Q = Q_{\mathbf{R}} \left[\int_{-\infty}^{B_0} d\xi \rho^{(0)}(\xi) - 3 \int_{-\infty}^{B_{12}} d\xi \rho^{(12)}(\xi) \right], \quad \Delta > 0,$$
$$Q = Q_{\mathbf{R}} \left[3 \int_{-\infty}^{B_2} d\xi \rho^{(2)}(\xi) - \int_{-\infty}^{B_{14}} d\xi \rho^{(14)}(\xi) \right], \quad \Delta < 0,$$
(32)

where $Q_{\mathbf{R}} = 16$ for $\mathbf{R} \| (1,0,0)$, $Q_{\mathbf{R}} = -4$ for $\mathbf{R} \| (1,1,1)$, and $Q_{\mathbf{R}} = 32/7$ for $\mathbf{R} \| (1,1,0)$.

The quadrupolar moment of the pair of impurities is shown in Fig. 5 as a function of Δ/T_K for the three principal directions. Note that for $\Delta = 0$ the quadrupolar moment vanishes, indicating that the RKKY interaction is necessary to induce a nonzero Q. Isolated impurities do not have a quadrupolar moment, because the Kondo effect screens all internal degrees of freedom, i.e., the spin and the orbital content of the Γ_8 quadruplet.

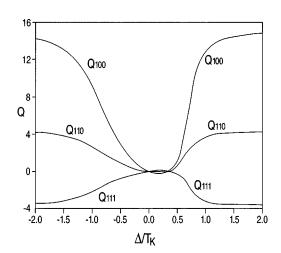


FIG. 5. Quadrupolar moment induced by the RKKY interaction as a function of Δ/T_K . The vector **R** joining the two impurities is along the (1,0,0), (1,1,0), and (1,1,1) directions of the crystal.

V. CONCLUDING REMARKS

We considered an interacting pair of Ce ions embedded into LaB₆. Each Ce impurity has a Γ_8 ground quartet that interacts with the conduction states via a Kondo exchange potential of the Coqblin-Schrieffer type. The band structure of the alloy Ce_xLa_{1-x}B₆ close to the Fermi surface consists of three ellipsoidal pockets centered at the *X* points of the simple cubic Brillouin zone. This band picture is not changed with the Ce concentration for the entire range of *x* ($0 \le x \le 1$). The Kondo exchange interaction involves these three anisotropic bands, and through this exchange interaction a conduction electron annihilated in one pocket may reappear in another pocket.

The conduction states mediate the RKKY interaction between the Ce sites. All three pockets contribute and give rise to an interference effect, which is constructive for sites separated by a vector **R** whose components are either all even or all odd multiples of the cubic lattice constant *a*. This constructive interference yields an enhancement factor of 9 as compared to all other **R** vectors. The strongly coupled sites form a super-bcc-lattice of lattice constant 2a.

The anisotropy of each of the pockets does not give rise to any dramatic effect. Leaving aside the interference factor between the pockets, the anisotropy yields an $|\mathbf{R}|$ dependence of the RKKY interaction that is no longer spherical but has cubic symmetry.

The 16 states of a pair of Ce impurities with Γ_8 ground multiplet are split by the RKKY interaction into a singlet, a twelvefold degenerate multiplet, and a triplet. This is the case independently of the direction of **R** relative to the crystal axis. The amplitude of the interaction and the linear combination of states splitting into the singlet and triplet of course depend on the relative direction of **R** to the crystal axis.

The exact solution of a model for a pair of interacting Kondo impurities with a Γ_8 ground multiplet¹⁶ was used to explore the consequences of the RKKY splitting into a singlet, a twelvefold degenerate multiplet, and a triplet. The main assumptions (described in detail in Sec. II of Ref. 16) leading to the integrable two-impurity model (18) are: (i) electrons are considered in pairs, so that either both impurities have one localized electron or both are in the empty configuration, (ii) the conduction states interacting with the impurity are considered in two channels (e.g., even and odd parity states with respect to the midpoint between the impurities), (iii) both channels interact with the impurities via a contact potential, (iv) the pairs of conduction electrons are not allowed to break up and recombine in a different way. i.e., they are assumed to be hard-core bosons, and finally (v) the RKKY interaction is incorporated *a posteriori* as a splitting of the sixteenfold multiplet.

As a function of Δ/T_K we studied the population of the impurity levels, the magnetic susceptibility for $\mathbf{R} \parallel (1,0,0)$ and (1,1,1), the linear temperature coefficient γ of the specific heat, the Wilson ratio and the quadrupolar moment Q. Due to the Kondo effect, the ground state is always a magnetic singlet. The magnetic susceptibility falls off rapidly with Δ/T_K if the impurities are antiferromagnetically correlated, while it increases with a power law for ferromagnetic RKKY. Here the impurities lock into a triplet, which

is then spin compensated by the Kondo effect. Such a power-law dependence was found previously in the context of orbital quenching by crystalline fields and spin-orbit splitting in the Coqblin-Schrieffer model.^{21–23} The dependence of χ^s_{imp} on Δ/T_K is different from that of S = 1/2 impurities because of the presence of the twelvefold multiplet.

There are two types of contributions to the specific heat γ coefficient. The spin fluctuations of the triplet and the twelvefold multiplet yielding χ^s_{imp} also contribute to γ . In addition there are two terms arising from the thermal population fluctuations of the RKKY-split states, which are largest for $|\Delta| \approx T_K$. For antiferromagnetic RKKY coupling, γ decreases rapidly for large Δ/T_K because the impurities compensate each other, while for $\Delta < 0$ the coefficient increases as a consequence of the Kondo effect of the triplet. The dependence of the Wilson ratio on Δ is a manifestation of the nonuniversality of the two-impurity Kondo problem.

As a consequence of the RKKY splitting into a singlet, a twelvefold degenerate multiplet, and a triplet, a quadrupolar moment is induced. Such a nonzero expectation value of the quadrupolar moment is absent in the single impurity case. The quadrupolar moment is larger for **R** parallel to the (1,0,0) direction than in the (1,1,0) and (1,1,1) directions. *Q* is positive along (1,0,0) and (1,1,0), but negative along (1,1,1).

The hybridization of the conduction states with the impurity states eliminates the particle-hole symmetry from the start, so that our model always yields Fermi-liquid-like properties, displaying nonuniversal behavior as a function of Δ/T_K , as expected from a line of fixed points joining the end points $\Delta \rightarrow \pm \infty$. The unstable fixed point with non-Fermi-liquid properties found in Ref. 8 is bypassed.

In Sec. I we motivated this study with the rich phase diagram of the alloy series $(Ce_rLa_{1-r})B_6$. Although it is speculative to extrapolate from the solution of the two-site problem on the properties of a lattice of Ce ions, we will attempt an explanation of the antiferroquadrupolar order of CeB_6 . Due to the interference of the three electron pockets, the interaction is strongest among sites on super-bcc-lattice of lattice constant 2a. The simple cubic lattice of (Ce,La) ions can be subdivided into four such interpenetrating superbcc-lattices. The corners on each of a bcc-lattice cube are ferroquadrupolarly ordered [(1,0,0)] direction, while the body-centered ions are antiferroquadrupolarly ordered with respect to the corners [(1,1,1) direction]. The relative order of the super-bcc-lattices among each other is determined by the dominating ferroquadrupolar correlation between from the corners to the centers of the faces [(1,1,0)] direction]. Here we assumed that the RKKY interaction is short ranged. This leads to an overall antiferroquadrupolar order of wave vector $\mathbf{k}_0 = (1,1,1)(\pi/a)$ as observed experimentally.24

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